

Subtleties in Quantum Mechanical Metastability

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We present a detailed discussion of some features of quantum mechanical metastability. We analyze the nature of decaying (quasistationary) states and the regime of validity of the exponential law, as well as decays at finite temperature. We resort to very simple systems and elementary techniques to emphasize subtle aspects of the problem.

I. INTRODUCTION

Complex-energy eigenfunctions made their début in Quantum Mechanics through the hands of Gamow, in the theory of alpha-decay.¹ Gamow imposed an “outgoing wave boundary condition” on the solutions of the Schrödinger equation for an alpha-particle trapped in the nucleus. Since there is only an *outgoing* flux of alpha-particles, the wave function $\psi(r, t)$ must behave far from the nucleus as (for simplicity, we consider an s-wave)²

$$\psi(r, t) \sim \frac{e^{-iEt+ikr}}{r} \quad (r \rightarrow \infty). \quad (1)$$

This boundary condition, together with the requirement of finiteness of the wave function at the origin, gives rise to a quantization condition on the values of k (and, therefore, on the values of $E = k^2/2$). It turns out that such values are complex:

$$k_n = \kappa_n - iK_n/2, \quad E_n = \epsilon_n - i\Gamma_n/2. \quad (2)$$

It follows that

$$|\psi_n(r, t)|^2 \sim \frac{e^{-\Gamma_n t + K_n r}}{r^2} \quad (r \rightarrow \infty). \quad (3)$$

Thus, if $\Gamma_n > 0$, the probability of finding the alpha-particle in the nucleus decays exponentially in time. The lifetime of the nucleus would be given by $\tau_n = 1/\Gamma_n$, and the energy of the emitted alpha-particle by ϵ_n .

Although very natural, this interpretation suffers from some difficulties. How can the energy, which is an observable quantity, be complex? In other words, how can the Hamiltonian, which is a Hermitean operator, have complex eigenvalues? Also, the eigenfunctions are not normalizable, since Γ_n positive implies K_n positive and, therefore, according to (3), $|\psi_n(r, t)|^2$ diverges exponentially with r .

In spite of such problems (which, in fact, are closely related), it is a fact of life that alpha-decay, as well as other types of decay, does obey an exponential decay law, with a rate close to that obtained using Gamow's

method. Why this method works is the question we try to answer in this paper in a very elementary way.³ Thus, in Section II, we show Gamow's method in action for a very simple potential. Some of the results obtained there are used in Section III, where we study the time evolution of a wave packet initially confined in the potential well defined in Section II. This is done with the help of the propagator built with normalizable⁴ eigenfunctions, associated to real eigenenergies. As a bonus, we show that the exponential decay law is not valid for very small times or for very large times. This is the content of Section IV, where the region of validity of the exponential decay law is roughly delimited.

Another topic we address in this paper is decay at finite temperature. This is done in Section V, where we study, with the help of an exactly solvable toy model, how the decay of a metastable system is modified when it is coupled to a heat bath. It is shown that, under suitable conditions, the decay is exponential, with a decay rate Γ given by the thermal average of the Γ_n 's,

$$\Gamma = \frac{\sum_n \Gamma_n e^{-\beta \epsilon_n}}{\sum_n e^{-\beta \epsilon_n}}. \quad (4)$$

Although this result appears to be rather obvious, in fact it is not: the decay of a metastable system is an intrinsically non-equilibrium process and, so, there is no a priori reason for the decay rate to be given by (4). Finally, in Section VI, we discuss the concept of “free energy of a metastable phase,” a point where we think there is some confusion in the literature.

The results and ideas presented here are not really new, but discussions on these matters usually involve the use of sophisticated mathematical techniques, such as functional^{5,6} or complex analysis.⁷⁻¹¹ For this reason, we have tried to make the presentation as clear as possible by resorting to very simple systems and elementary techniques — in fact, techniques that can be found in any standard Quantum Mechanics textbook.¹²

II. DECAYING STATES

In order to exhibit Gamow's method in action, we shall study the escape of a particle from the potential well given by:

$$V(x) = \begin{cases} (\lambda/a) \delta(x-a) & \text{for } x > 0, \\ +\infty & \text{for } x < 0. \end{cases} \quad (5)$$

Motion in the region $x < 0$ is forbidden because of the infinite wall at the origin. The positive dimensionless constant λ is a measure of the "opacity" of the barrier at $x = a$; in the limit $\lambda \rightarrow \infty$, the barrier becomes impenetrable, and the energy levels inside the well are quantized. If λ is finite, but very large, a particle is no more confined to the well, but it usually stays there for a long time before it escapes. If λ is not so large, the particle can easily tunnel through the barrier, and quickly escape from the potential well. Metastability, therefore, can only be achieved if the barrier is very opaque, i.e., λ is very large. For this reason, we shall assume this to be the case in what follows and, whenever possible, we shall retain only the first non-trivial term in a $1/\lambda$ expansion.

To find out how fast the particle escapes from the potential well, we must solve the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(x, t) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \psi(x, t) + \frac{\lambda}{a} \delta(x-a) \psi(x, t). \quad (6)$$

$\psi(x, t) = \exp(-iEt) \varphi(x)$ is a particular solution of this equation, provided $\varphi(x)$ satisfies the time-independent Schrödinger equation

$$-\frac{1}{2} \frac{d^2}{dx^2} \varphi(x) + \frac{\lambda}{a} \delta(x-a) \varphi(x) = E \varphi(x). \quad (7)$$

Denoting the regions $0 < x < a$ and $x > a$ by the indices 1 and 2, respectively, the corresponding wave functions $\varphi_j(x)$ ($j = 1, 2$) satisfy the free-particle Schrödinger equation:

$$-\frac{1}{2} \frac{d^2}{dx^2} \varphi_j(x) = E \varphi_j(x). \quad (8)$$

Since the wall at the origin is impenetrable, $\varphi_1(0)$ must be zero; the solution of Eq. (8) which obeys this boundary condition is

$$\varphi_1(x) = A \sin kx \quad (k = \sqrt{2E}). \quad (9)$$

To determine $\varphi_2(x)$, we follow Gamow's reasoning^{1,6,13} and require $\varphi_2(x)$ to be an outgoing wave. Therefore, we select, from the admissible solutions of Eq. (8),

$$\varphi_2(x) = B e^{ikx}. \quad (10)$$

The wave function must be continuous at $x = a$, so that $\varphi_1(a) = \varphi_2(a)$, or

$$\frac{B}{A} = e^{-ika} \sin ka. \quad (11)$$

On the other hand, the derivative of the wave function has a discontinuity at $x = a$, which can be determined by integrating both sides of (7) from $a - \varepsilon$ to $a + \varepsilon$, with $\varepsilon \rightarrow 0^+$:

$$\varphi_2'(a) - \varphi_1'(a) = \frac{2\lambda}{a} \varphi_2(a), \quad (12)$$

from which there follows another relation between A and B :

$$\frac{B}{A} = \frac{e^{-ika} \cos ka}{i - 2\lambda/ka}. \quad (13)$$

Combining (11) and (13), we obtain a quantization condition for k :

$$\cotan ka = i - \frac{2\lambda}{ka}. \quad (14)$$

The roots of Eq. (14) are complex; when $\lambda \gg 1$, those which are closest to the origin are given by⁸

$$k_n \approx \frac{1}{a} \left[\frac{2n\pi\lambda}{1+2\lambda} - i \left(\frac{n\pi}{2\lambda} \right)^2 \right] \quad (n\pi \ll \lambda) \quad (15)$$

$$\equiv \kappa_n - iK_n/2.$$

The corresponding eigenenergies are

$$E_n = k_n^2/2 \approx \frac{1}{2} \left(\frac{n\pi}{a} \right)^2 - i \frac{(n\pi)^3}{(2\lambda a)^2} \quad (16)$$

$$\equiv \epsilon_n - i\Gamma_n/2.$$

(Note that $K_n \ll \kappa_n$ and $\Gamma_n \ll \epsilon_n$; these results will be used later.) The imaginary part of E_n gives rise to an exponential decay of $|\psi_n(x, t)|^2$, with lifetime equal to

$$\tau_n = 1/\Gamma_n \approx \frac{2(\lambda a)^2}{(n\pi)^3}. \quad (17)$$

Since the corresponding value of B/A is very small ($\sim n/\lambda$), one may be tempted to say that the probability of finding the particle outside the well is negligible in comparison with the probability of finding the particle inside the well. Normalizing ψ_n in such a way that the latter equals one when $t = 0$, the probability of finding the particle inside the well at time t , if it were in the n -th decaying state at $t = 0$, would be

$$P_n(t) = \int_0^a |\psi_n(x, t)|^2 dx = \exp(-\Gamma_n t). \quad (18)$$

The trouble with this interpretation is that $\text{Im } k_n \equiv -K_n/2 < 0$, and so $\psi_n(x, t)$ diverges exponentially as $x \rightarrow \infty$, since, according to (10),

$$|\psi_n(x, t)|^2 = |B_n|^2 \exp(-\Gamma_n t + K_n x) \quad (19)$$

outside the well. Because of this "exponential catastrophe", the decaying states are nonnormalizable and, therefore, cannot be accepted as legitimate solutions of the Schrödinger equation (although one can find in the literature the assertion that they are "rigorous" solutions of the time-dependent Schrödinger equation¹⁴).

III. TIME EVOLUTION OF A WAVE PACKET

We now return to Eq. (8) and write, for the solution in region 2, instead of (10), the sum of an outgoing plus an incoming wave:

$$\varphi_2(x) = e^{-ikx} + B e^{ikx}. \quad (20)$$

Continuity of the wave function at $x = a$ implies

$$A \sin ka = e^{-ika} + B e^{ika}. \quad (21)$$

As before, the derivative of the wave function has a discontinuity at $x = a$, given by Eq. (12), from which it follows, instead of (13),

$$kA \cos ka = -\left(\frac{2\lambda}{a} + ik\right) e^{-ika} - \left(\frac{2\lambda}{a} - ik\right) B e^{ika}. \quad (22)$$

Solving (21) and (22) for A and B , we find

$$A = -\frac{2ika}{(ka + \lambda \sin 2ka) + i2\lambda \sin^2 ka}, \quad (23a)$$

$$B = -\frac{(ka + \lambda \sin 2ka) - i2\lambda \sin^2 ka}{(ka + \lambda \sin 2ka) + i2\lambda \sin^2 ka}. \quad (23b)$$

These expressions show a couple of interesting features:

(1) $|B| = 1$ for real values of k , implying a zero net flux of probability through $x = a$; therefore, unlike the solution found in the previous section, there is no loss or accumulation of probability in the well region.

(2) $|A| \ll 1$ if $ka \ll \lambda$, except if k is close to a pole of $A(k)$, in which case $|A|$ may become very large.

To find the poles of A we must solve the equation $A(k)^{-1} = 0$, which, after some algebraic manipulations, reads

$$\cotan ka = i - \frac{2\lambda}{ka}. \quad (24)$$

This is the same as Eq. (14)! Is this a coincidence? In fact, no. According to (23), A and B have the same poles; in a sufficiently small vicinity of a pole, $|A|$ and $|B|$ are very large, and so Eqs. (21) and (22) become equivalent to Eqs. (11) and (13), respectively.

Suppose that at $t = 0$ the particle is known to be in the region $x < a$ with probability 1; in other words, its wave function $\psi(x, 0)$ is zero outside the well,

$$\psi(x, 0) = 0 \quad \text{for } x > a. \quad (25)$$

The wave function at a later time t is given by

$$\psi(x, t) = \int_0^a G(x, x'; t) \psi(x', 0) dx', \quad (26)$$

where the propagator, $G(x, x'; t)$, can be written as

$$G(x, x'; t) = \int_0^\infty e^{-ik^2 t/2} \varphi^*(k, x) \varphi(k, x') dk. \quad (27)$$

The function $\varphi(k, x)$ is the solution of Eq. (7) corresponding to the energy $E = k^2/2$:

$$\varphi(k, x) = \frac{1}{\sqrt{2\pi}} \times \begin{cases} A(k) \sin kx & (x < a) \\ e^{-ikx} + B(k) e^{ikx} & (x > a). \end{cases} \quad (28)$$

With this normalization, the $\varphi(k, x)$ satisfy the completeness relation¹⁵

$$\int_0^\infty \varphi^*(k, x) \varphi(k, x') dk = \delta(x - x'). \quad (29)$$

Since, by hypothesis, $\psi(x, 0) = 0$ for $x > a$, (26)–(28) give, for $x < a$,

$$\begin{aligned} \psi(x, t) &= \frac{1}{2\pi} \int_0^\infty dk e^{-ik^2 t/2} |A(k)|^2 \sin kx \\ &\times \int_0^a dx' \psi(x', 0) \sin kx'. \end{aligned} \quad (30)$$

For k close to a pole $k_n \equiv \kappa_n - iK_n/2$, $A(k)$ can be approximated by

$$\begin{aligned} A(k) &\approx -\frac{2ik_n a}{a(1 + 2\lambda e^{2ik_n a})(k - k_n)} \\ &\approx -\frac{i\kappa_n/\lambda}{(k - \kappa_n) + iK_n/2}. \end{aligned} \quad (31)$$

As we have seen, $|A(k)|^2 \ll 1$ if $ka \ll \lambda$, except at the resonances, where (31) may be used. On the other hand, if $\psi(x, 0)$ is sufficiently smooth, in the sense that $\int_0^a dx \psi(x, 0) \sin kx \rightarrow 0$ sufficiently fast when $k \rightarrow \infty$ (this condition will be made more precise later), then most of the contribution to the integral (30) comes from the region $ka \ll \lambda$. Therefore, we may approximate (30) by

$$\begin{aligned} \psi(x, t) &\approx \frac{1}{2\pi} \sum_n \int_{I_n} dk e^{-ik^2 t/2} \frac{(\kappa_n/\lambda)^2 \sin kx}{(k - \kappa_n)^2 + K_n^2/4} \\ &\times \int_0^a dx' \psi(x', 0) \sin kx', \end{aligned} \quad (32)$$

where I_n is the interval $[(\kappa_n + \kappa_{n-1})/2, (\kappa_n + \kappa_{n+1})/2]$ ($n = 1, 2, \dots; \kappa_0 \equiv 0$). Because of the arguments preceding (32), only the first few terms of the sum give a significant contribution to the integral. Note also that, since the resonance in $|A(k)|^2$ around κ_n has a width of the order of K_n , and

$$K_n x, K_n x' \leq K_n a \approx (n\pi)^2/2\lambda^2 \ll 1, \quad (33)$$

we can substitute k for κ_n in $\sin kx$ and $\sin kx'$ in the integrand of (32). On the other hand, this is not allowed for $e^{-ik^2 t/2}$, since the time t is not bounded.

Let us examine the integrals

$$\mathcal{I}_n(t) \equiv \int_{I_n} dk e^{-ik^2 t/2} \frac{1}{(k - \kappa_n)^2 + K_n^2/4}. \quad (34)$$

If $K_n \ll \kappa_{n+1} - \kappa_{n-1}$, we can safely extend the interval of integration to the whole real axis, and carrying out the integration we find

$$\begin{aligned} \mathcal{I}_n(t) &\approx \int_{-\infty}^{\infty} dk e^{-ik^2 t/2} \frac{1}{(k - \kappa_n)^2 + K_n^2/4} \\ &= \frac{1}{\sqrt{2\pi i t}} \int_{-\infty}^{\infty} d\xi e^{i\xi^2/2t} \int_{-\infty}^{\infty} \frac{dk e^{i\xi k}}{(k - \kappa_n)^2 + K_n^2/4} \\ &= \frac{2\pi}{K_n \sqrt{2\pi i t}} (\mathcal{I}_n^1 + \mathcal{I}_n^2); \end{aligned} \quad (35a)$$

$$\mathcal{I}_n^1 \equiv \int_{-\infty}^0 d\xi e^{i\xi^2/2t + i(\kappa_n - iK_n/2)\xi}, \quad (35b)$$

$$\mathcal{I}_n^2 \equiv \int_0^{\infty} d\xi e^{i\xi^2/2t + i(\kappa_n + iK_n/2)\xi}. \quad (35c)$$

Except for a region of width $\Delta\xi \sim \sqrt{t}$ around the point $\xi = -\kappa_n t$, where the phases of the exponentials are stationary, the oscillations of the integrands tend to cancel out, giving a very small contribution to the integrals above. If $\kappa_n t \gg \sqrt{t}$, such a region is well inside the negative real axis, therefore the second integral can be neglected in comparison to the first. For the same reason, we can extend the interval of integration of the first integral to the whole real axis, thus obtaining

$$\begin{aligned} \mathcal{I}_n(t) &\approx \frac{2\pi}{K_n \sqrt{2\pi i t}} \int_{-\infty}^{\infty} d\xi e^{i\xi^2/2t + i(\kappa_n - iK_n/2)\xi} \\ &= \frac{2\pi}{K_n} e^{-i(\kappa_n - iK_n/2)^2 t/2} = \frac{2\pi}{K_n} e^{-iE_n t}. \end{aligned} \quad (36)$$

Substituting this result in Eq. (32), we find

$$\psi(x, t) \approx \sum_n c_n e^{-iE_n t} \varphi_n(x), \quad (37)$$

where $\varphi_n(x)$ and c_n are defined as

$$\varphi_n(x) = \sqrt{\frac{a}{2}} \frac{(\kappa_n/\lambda)^2}{K_n} \sin \kappa_n x \approx \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad (38a)$$

$$c_n = \int_0^a dx \psi(x, 0) \varphi_n(x). \quad (38b)$$

Eq. (37) is formally identical to the well known expansion of the wave function in energy eigenfunctions, except for the fact that: (1) it is an *approximate* result and, as such, subject to some restrictions, and (2) the energies E_n are complex, as a result of which the probability $P(t)$ to find the particle inside the potential well at time t decreases in time:

$$P(t) = \int_0^a |\psi(x, t)|^2 dx \approx \sum_n |c_n|^2 e^{-\Gamma_n t}. \quad (39)$$

Now we can be more precise on the smoothness of $\psi(x, 0)$; roughly speaking, the smaller the value of n beyond which $c_n = 0$, the better the results above will be.

Eq. (37) is valid only inside the potential well. To find the wave function outside the well, we must return to Eqs. (26)–(28) and make $x > a$:

$$\begin{aligned} \psi(x, t) &= \frac{1}{2\pi} \int_0^{\infty} dk e^{-ik^2 t/2} [e^{ikx} + B^*(k) e^{-ikx}] A(k) \\ &\times \int_0^a dx' \psi(x', 0) \sin kx'. \end{aligned} \quad (40)$$

Since most of the contribution to the integral in k comes from the resonances, we may approximate $A(k)$ by (31) and make an analogous approximation for $B^*(k)$. Thus, (40) becomes

$$\psi(x, t) \approx \sum_n d_n \mathcal{J}_n(x, t); \quad (41a)$$

$$d_n \equiv \frac{-i\kappa_n}{2\pi\lambda} \int_0^a dx' \psi(x', 0) \sin \kappa_n x', \quad (41b)$$

$$\mathcal{J}_n(x, t) \equiv \int_{I_n} dk e^{-ik^2 t/2} \left(\frac{e^{ikx}}{k - \kappa_n + iK_n/2} - \text{c.c.} \right). \quad (41c)$$

where I_n has the same meaning as in Eq. (32), and c.c. denotes complex conjugate.

Let us concentrate our attention on the integrals $\mathcal{J}_n(x, t)$. Extending the interval of integration to the whole real axis, and using the same trick as in Eq. (35a), we find

$$\mathcal{J}_n(x, t) \approx -\frac{2\pi i}{\sqrt{2\pi i t}} (\mathcal{J}_n^1 + \mathcal{J}_n^2); \quad (42a)$$

$$\mathcal{J}_n^1 \equiv \int_{-\infty}^{-x} d\xi e^{i\xi^2/2t + i\kappa_n(\xi+x)}, \quad (42b)$$

$$\mathcal{J}_n^2 \equiv \int_x^{\infty} d\xi e^{i\xi^2/2t + i\kappa_n^*(\xi-x)}. \quad (42c)$$

As in the case of $\mathcal{I}_n(t)$, the second integral is negligible in comparison to the first if $\kappa_n t \gg \sqrt{t}$, or $t \gg 1/\epsilon_n$. On the other hand, the first integral may be approximated by

$$\int_{-\infty}^{\infty} d\xi e^{i\xi^2/2t + i\kappa_n(\xi+x)} = \sqrt{2\pi i t} e^{-ik_n^2 t/2 + i\kappa_n x} \quad (43)$$

only if $\kappa_n t - x \ll \sqrt{t}$.

Returning to Eq. (41), we finally obtain

$$\psi(x, t) \approx -2\pi i \sum_n d_n e^{-iE_n t + i\kappa_n x}. \quad (44)$$

We see, therefore, that outside the well the wavefunction behaves as a superposition of outgoing waves, in the way postulated by Gamow. However, the exponential catastrophe does not occur here, for Eq. (44) is valid only under the assumption that $\kappa_n t - x \ll \sqrt{t}$.

IV. BREAKDOWN OF EXPONENTIAL DECAY

The evolution of the wave function requires some time¹⁷ to reach the regime of exponential decay; typically, a time corresponding to many oscillations inside the potential well (i.e., $t \gg 1/\epsilon_n$). To be more precise, even if this condition is satisfied, the decay is not strictly exponential, but a sum of exponential decays, one for each resonance [Eq. (39)]. However, since the lifetime τ_n is, in general, a rapidly decreasing function of n ($\tau_n \approx \tau_1/n^3$ in our example), the decay becomes a pure exponential one after a time of the order of τ_1 .

On the other hand, the exponential decay does not last forever. After some sufficiently long time, it obeys a power law.^{7-11,16} To see this, note that for $t \rightarrow \infty$, the integral (30) is dominated by small values of k . One finds, then, for $x < a$,

$$\begin{aligned} \psi(x, t) &\approx \frac{|A(0)|^2 x}{2\pi} \int_0^a dx' \psi(x', 0) x' \int_0^\infty dk e^{-ik^2 t/2} k^2 \\ &= \frac{x}{\lambda^2 \sqrt{8\pi i t^3}} \int_0^a dx' \psi(x', 0) x'. \end{aligned} \quad (45)$$

Therefore, the probability of finding the particle inside the potential well behaves asymptotically as

$$P(t) \approx \frac{a^3}{24\pi\lambda^4 t^3} \left| \int_0^a dx' \psi(x', 0) x' \right|^2 \sim \frac{a^6}{\lambda^4 t^3}. \quad (46)$$

Comparing (46) with (39), one finds that they become comparable in magnitude when

$$e^{-t/\tau_1} \sim \frac{a^6}{\lambda^4 t^3} \sim \lambda^{-10} \left(\frac{\tau_1}{t} \right)^{-3}, \quad (47)$$

or, since $\lambda \gg 1$,

$$\frac{t}{\tau_1} \sim 10 \ln \lambda + 3 \ln \ln \lambda. \quad (48)$$

Thus, when the decay begins to obey a power law¹⁸ ($\sim t^{-3}$), the probability that the particle is still inside the potential well is so small ($\lesssim \lambda^{-10}$), that it would be very difficult to observe deviations from the exponential decay.

V. DECAY AT FINITE TEMPERATURE

In general, the initial state of the particle, $\psi(x, 0)$, is not precisely known. Such a knowledge is required in order to determine the coefficients c_n in Eq. (37). Let us imagine, however, that the system is in contact with a heat bath at temperature T . Then, it is reasonable to assume that ($\beta = 1/k_B T$, k_B = Boltzmann constant)

$$|c_n|^2 = \frac{e^{-\beta\epsilon_n}}{Z}, \quad Z \equiv \sum_n e^{-\beta\epsilon_n}. \quad (49)$$

Thus, Eq. (37) gives

$$P(t) \approx \frac{1}{Z} \sum_n e^{-\beta\epsilon_n - \Gamma_n t}, \quad (50)$$

and, as already discussed in Sec. IV, after a time of the order $\tau_1 = 1/\Gamma_1$, the decay would be dominated by the decay of the “false vacuum” — the lowest lying resonance. It follows that the decay rate is almost insensitive to the temperature.

Is this conclusion correct?

In the literature¹⁹ one finds the statement that, in such a situation, the probability $P(t)$ decays as

$$P(t) = e^{-\langle \Gamma \rangle t}, \quad \langle \Gamma \rangle = \frac{1}{Z} \sum_n \Gamma_n e^{-\beta\epsilon_n}. \quad (51)$$

A perfectly sensible question is: why does $P(t)$ decay this way, and not as

$$P(t) = e^{-t/\langle \tau \rangle}, \quad \langle \tau \rangle = \frac{1}{Z} \sum_n \tau_n e^{-\beta\epsilon_n} ? \quad (52)$$

In order to answer these questions, we shall study a toy model: a two-level metastable system coupled to a heat bath. (For instance, imagine a situation in which only the two lowest resonances of a potential well are excited.) These levels have “complex energies” $E_j = \epsilon_j - i\Gamma_j/2$ ($j = 1, 2$). Let $n_1(t)$ and $n_2(t)$ be the populations at time t of levels 1 and 2, respectively. A reasonable dynamics is given by the following set of equations ($\dot{n} \equiv dn/dt$, $E \equiv \epsilon_2 - \epsilon_1$):

$$\begin{cases} \dot{n}_1 = -\Gamma_1 n_1 + \Gamma (n_2 - e^{-\beta E} n_1), \\ \dot{n}_2 = -\Gamma_2 n_2 - \Gamma (n_2 - e^{-\beta E} n_1). \end{cases} \quad (53)$$

The first term on the r.h.s. of (53) describes the “natural” decay of the levels. The second term is due to the coupling to the heat bath; it drives the system towards thermal equilibrium with the bath.

Since (53) is a set of differential linear equations, solutions can be found in the form

$$n_1(t) = a e^{-\lambda t}, \quad n_2(t) = b e^{-\lambda t}. \quad (54)$$

The decay rate, λ , must satisfy the characteristic equation

$$\begin{aligned} \lambda^2 - [\Gamma_1 + \Gamma_2 + (1 + e^{-\beta E})\Gamma] \lambda \\ + \Gamma_1 \Gamma_2 + (\Gamma_1 + e^{-\beta E} \Gamma_2) \Gamma = 0. \end{aligned} \quad (55)$$

Although this equation can be solved exactly, the exact solution is not very illuminating. Instead, we shall consider two limiting situations.

(1) $\Gamma \gg \Gamma_1, \Gamma_2$ (overdamping): in this case, we may approximate Eq. (55) by

$$\lambda^2 - (1 + e^{-\beta E})\Gamma \lambda + (\Gamma_1 + e^{-\beta E} \Gamma_2) \Gamma = 0, \quad (56)$$

whose solutions are

$$\lambda_{\pm} = \frac{1}{2}(1 + e^{-\beta E})\Gamma \left(1 \pm \sqrt{1 - \frac{4(\Gamma_1 + e^{-\beta E}\Gamma_2)}{(1 + e^{-\beta E})^2\Gamma}} \right). \quad (57)$$

Expanding the square root, we find (since $\Gamma_1, \Gamma_2 \ll \Gamma$)

$$\lambda_+ \approx (1 + e^{-\beta E})\Gamma, \quad (58a)$$

$$\lambda_- \approx \frac{\Gamma_1 + e^{-\beta E}\Gamma_2}{1 + e^{-\beta E}} \equiv \langle \Gamma \rangle. \quad (58b)$$

The corresponding eigenvectors are

$$\begin{pmatrix} a_+ \\ b_+ \end{pmatrix} \approx \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} a_- \\ b_- \end{pmatrix} \approx \begin{pmatrix} 1 \\ e^{-\beta E} \end{pmatrix}. \quad (59)$$

If $n_j(0) = n_{j0}$ ($j = 1, 2$), then, at time t , we have

$$\begin{pmatrix} n_1(t) \\ n_2(t) \end{pmatrix} \approx \frac{e^{-\beta E} n_{10} - n_{20}}{1 + e^{-\beta E}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{-\lambda_+ t} + \frac{n_{10} + n_{20}}{1 + e^{-\beta E}} \begin{pmatrix} 1 \\ e^{-\beta E} \end{pmatrix} e^{-\lambda_- t}. \quad (60)$$

Therefore, even if the system is initially not in thermal equilibrium with the heat bath, it thermalizes in a time of the order $1/\lambda_+ \ll 1/\lambda_-$. In other words, after a transient time of the order of $1/\lambda_+$, both levels decay at the same rate, λ_- , equal to the thermal average of Γ_1 and Γ_2 , and their populations soon approach the Boltzmann distribution,

$$\frac{n_2(t)}{n_1(t)} \approx e^{-\beta E}. \quad (61)$$

(2) $\Gamma \ll \Gamma_1, \Gamma_2$ (underdamping): now, Eq. (55) may be approximated by

$$\lambda^2 - (\Gamma_1 + \Gamma_2)\lambda + \Gamma_1\Gamma_2 = 0, \quad (62)$$

whose solutions are $\lambda_j = \Gamma_j$ ($j = 1, 2$). The corresponding eigenvectors are²⁰

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \approx \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \approx \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (63)$$

The solution of (53) is, therefore,

$$n_j(t) \approx n_{j0} e^{-\Gamma_j t} \quad (j = 1, 2). \quad (64)$$

In this case, the levels decouple from each other, and each one of them decays with its own decay rate. The coupling to the heat bath is so weak that the system is effectively insulated.

Now we are in position to answer the questions posed in this section:

(A) If the system is overdamped (i.e., $\Gamma \gg \Gamma_1, \Gamma_2$), it decays as indicated in (51). The analysis of the overdamped case also explains why the decay rate is given

by (51), instead of (52). (In some sense, that is why one can observe a phenomenon like the Stark effect. In the presence of a constant external electric field, the potential which binds an electron to an atom becomes unbounded from below, and so the atomic energy levels become metastable, with very large lifetimes if the external electric field is small compared to the field of the nucleus. The role of the heat bath is played here by the quantized electromagnetic field; it is the coupling of the atom to it that causes the excited states of the atom, otherwise stationary, to decay to the ground state. Even for a highly excited atom, for which the natural lifetime is relatively high (some milliseconds), the situation is well described by saying that the atom is overdamped, since the ionization (decay) rate is very small if the external electric field is small compared to the intratomic field.)

(B) On the other hand, if the system is underdamped ($\Gamma \ll \Gamma_1, \Gamma_2$), although the decay is still described by Eq. (37), Eq. (50) is possibly not valid. The reason is that, under such a condition, the system does not “know” the temperature of the heat bath. It would have decayed before it could thermalize. In practice, as already argued, the excited states would depopulate much sooner than the “ground state,” and so the decay rate would be very insensitive to the temperature of the heat bath.

VI. THERMODYNAMICS OF METASTABLE SYSTEMS: A BRIEF DIGRESSION

Finally, we would like to make a brief digression on a point where we think there is some confusion in the literature. It concerns the thermodynamics of metastable systems. As an example of such a system, let us consider a particle interacting with the potential defined in Section II. Its partition function is defined as

$$\begin{aligned} \mathcal{Z} &\equiv \text{Tr } e^{-\beta H} \\ &= \int_0^\infty dk e^{-\beta k^2/2} \int_0^\infty dx \varphi^*(k, x) \varphi(k, x), \end{aligned} \quad (65)$$

or, alternatively, as

$$\mathcal{Z} = \int_0^\infty \rho(E) e^{-\beta E} dE. \quad (66)$$

Clearly, the spectral density $\rho(E)$ is given, in this case, by⁴

$$\rho(E) = \delta(0) \frac{dk}{dE} = \frac{\delta(0)}{\sqrt{2E}}. \quad (67)$$

We conclude, therefore, that there is no sign of metastability in the partition function. Now, let us try to define a “partition function inside the well;” since this is not a fundamental concept, more than one definition is possible. One such definition is inspired by (65); restricting the x -integration to the interval $[0, a]$, we have

$$Z_1 = \int_0^\infty dk e^{-\beta k^2/2} \int_0^a dx \varphi^*(k, x) \varphi(k, x). \quad (68)$$

If we make the same approximations we made in Section III, we can reexpress Z_1 as in (66), but now with a spectral density given by

$$\rho_1(E) \approx \sum_n \frac{1}{\pi} \frac{\Gamma_n/2}{(E - \epsilon_n)^2 + \Gamma_n^2/4}. \quad (69)$$

This kind of spectral density^{16,21} contains some dynamical information — resonant levels and decay rates. If the latter are small enough, the Lorentzians in (69) can be approximated by delta functions, and we obtain, therefore,

$$Z_1 \approx \sum_n e^{-\beta \epsilon_n} \equiv e^{-\beta F_1}. \quad (70)$$

If the coupling with the heat bath is strong (in the sense of Section V), F_1 can be interpreted^{22,23} as the free energy of the metastable phase. One should not confuse²¹ this “free energy” with the true equilibrium free energy, $\mathcal{F} = -(1/\beta) \ln Z$.

Another possible definition of the “partition function inside the well” is inspired in the complex eigenenergies of Gamow’s method:

$$Z_2 \equiv \sum_n e^{-\beta(\epsilon_n - i\Gamma_n/2)} \equiv e^{-\beta F_2}. \quad (71)$$

This definition, although almost identical to (70), presents a new and interesting feature: the free energy F_2 of the metastable phase is complex! Its real part is essentially equal to F_1 , and so has thermodynamical content, but its imaginary part provides dynamical information: if the Γ_n ’s are small, it is easy to show that

$$\text{Im } F_2 \approx -\frac{i}{2} \langle \Gamma \rangle, \quad (72)$$

where $\langle \Gamma \rangle$ is the thermal average of the Γ_n ’s, as defined in (51). That is the reason why definition (71) is so popular in the literature, although it is no more fundamental than definition (68).

VII. CONCLUSION

In Section III we showed that decaying states, although plagued by the exponential catastrophe, give a fairly good description of the decay of a metastable state, provided some conditions are satisfied. In fact, the main result of this paper is that one can compute the decay rate solving the time independent Schrödinger equation subject to the “outgoing wave boundary condition,” Eq. (10). This is far from being a trivial result, since the corresponding eigenstates are nonphysical. The “effectiveness” of the decaying states in describing the decay

may be understood by noticing⁵ that they are good approximate solutions to the time-dependent Schrödinger equation, although nonuniform ones (i.e., they are not valid in the entire range of values of t and x).

In Section V we examined another “well known” result, that the decay rate of a metastable system in contact with a heat bath is given by Eq. (51). Although we have used a very simple toy model to discuss this point, we believe it contains the essential physics of the phenomenon, at least in the two limiting cases we studied in some detail. The important lesson to be learned here is that Eq. (51) is correct (at least in first approximation), provided the condition of “overdamping” is satisfied.^{14,24} At low temperatures, where only the lowest lying decaying states take part in the process, it is an easy matter to verify if it is so. However, as the temperature increases, decaying states of higher energy are excited and begin to play an increasingly important role in the overall decay. Since the decay rates Γ_n become larger with n , the overdamping condition eventually fails to be satisfied by states actively involved in the process of decay. Thus, one should expect deviations from the decay rate given by Eq. (51). Another source of deviations, not taken into account in our toy model, is a possible renormalization of the complex energies E_n , caused by the interaction of the system with the heat bath. This may affect Eq. (51) even at low temperatures, for obvious reasons.²⁵

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² We use units such that $\hbar = m = 1$.

³ After this paper was written, we became aware of a paper by Barry Holstein, in which the content of Sections II and III is discussed using a more general potential. See B. R. Holstein, “Understanding alpha decay,” *Am. J. Phys.* **64**, 1061-1071 (1996).

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- ¹⁷ It can be shown^{9,10} that initially the decay is slower than exponential; more precisely, $dP/dt = 0$ when $t = 0$.
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